

ERROR ESTIMATES FOR APPROXIMATE SOLUTIONS OF THE RICCATI EQUATION WITH REAL OR COMPLEX POTENTIALS

FELIX FINSTER AND JOEL SMOLLER

JULY 2008

ABSTRACT. A method is presented for obtaining rigorous error estimates for approximate solutions of the Riccati equation, with real or complex potentials. Our main tool is to derive invariant region estimates for complex solutions of the Riccati equation. We explain the general strategy for applying these estimates and illustrate the method in typical examples, where the approximate solutions are obtained by glueing together WKB and Airy solutions of corresponding one-dimensional Schrödinger equations. Our method is motivated by and has applications to the analysis of linear wave equations in the geometry of a rotating black hole.

1. INTRODUCTION

The time-independent one-dimensional Schrödinger equation plays an important role in both mathematics and physics. Except in special situations, it is impossible to find exact solutions, and thus one resorts to approximation techniques. The most common method is to take the WKB wave functions away from the zeros of the potential, and to glue them together with Airy functions, which approximate the solutions near the zeros (see for example the textbook [9, Section 2.4] or the book [5]). Usually, the potential in the Schrödinger equation is real-valued. However, there are situations (like systems with dissipation) where the Schrödinger potential is complex.

The shortcoming of most approximation procedures is that they do not give error estimates. To quote Fröman and Fröman [5, page 3] (1965),

“In spite of the abundant literature there is still lacking a convenient method for obtaining definite limits of error. . . The problem of obtaining such limits of error is not only of academic or mathematical interest but is especially important in some physical applications. . .”

Unfortunately, such a convenient method for obtaining definite limits of error is still lacking today. Indeed, to our knowledge, despite the vast literature on WKB methods (see [4] and the references therein), only a few papers are concerned with rigorous error estimates. As typical examples see [7, 8], where L^2 -estimates are derived in the time-dependent setting for short times, as well as [6], where estimates are obtained in the setting of multiple tunneling. Here we shall develop a general method for obtaining *rigorous* pointwise error estimates for any given approximate solution in the time-independent setting, even in the case when the Schrödinger potential is complex.

We were led to the study of error estimates for solutions of one-dimensional Schrödinger equations from problems arising in general relativity. In particular, when analyzing

F.F. is supported in part by the Deutsche Forschungsgemeinschaft.

J.S. is supported in part by the Humboldt Foundation and the National Science Foundation, Grant No. DMS-0603754.

the scalar wave equation in the Kerr geometry, Carter's remarkable separation of variables [1] gives rise to a radial and angular ODE. These equations can both be transformed into the Schrödinger form, which are coupled through two parameters ω and λ . For estimating the global behavior of the solutions uniformly in ω and λ , we were led to the idea of using invariant disk estimates [3, 2]. When attempting to extend our analysis to gravitational waves in the framework of the Teukolsky equation [10], one of the difficulties that arises is that the potentials in the separated equations turn out to be complex. In the present paper, we obtain invariant disk estimates in a general setting, which are applicable to one-dimensional Schrödinger equations with a real or complex potential. The previous estimates in [3, 2] will arise as special cases. In particular, our method gives rigorous pointwise error estimates for the standard approximations by WKB and Airy functions. But the method works just as well for any other approximate solutions. The aim of the present paper is to introduce the method from a general point of view, and to illustrate it in typical examples. For an application to eigenvalue and gap estimates as well as to problems involving parameters we refer to [3] and [2].

We now set up the framework and fix our notation. The one-dimensional Schrödinger equation reads

$$\left[-\frac{d^2}{dx^2} + \mathcal{V}(x) \right] \phi(x) = \lambda \phi(x).$$

Absorbing the parameter λ into the potential, we rewrite the Schrödinger equation as

$$\frac{d^2}{dx^2} \phi = V(x) \phi(x), \quad (1.1)$$

where the new potential $V = \mathcal{V} - \lambda$ may depend on additional parameters. This is a linear second order ODE. Thus the general solution ϕ can be written as a linear combination of two linearly independent fundamental solutions ϕ_1 and ϕ_2 ,

$$\phi = a \phi_1 + b \phi_2. \quad (1.2)$$

By choosing the coefficients a and b appropriately, one can then satisfy suitable boundary conditions, if so desired. Setting

$$y = \frac{\phi'}{\phi}, \quad (1.3)$$

the function y satisfies the Riccati equation

$$y' = V - y^2. \quad (1.4)$$

Our strategy is to estimate y in the *complex plane*. This requires a brief explanation, because in the case when V is real it is natural to also choose ϕ , and thus y , to be real. This real function ϕ will in general have zeros, and y will be singular at each of these zeros. These divergences make it difficult to estimate y . We avoid this problem by considering a linear combination $\phi = \phi_1 + i\phi_2$ with real fundamental solutions ϕ_1 and ϕ_2 . Then, since the zeros of the fundamental solutions never coincide, the function ϕ never vanishes, and thus the corresponding function y is globally well-defined.

In the more general case when the potential V is complex, the situation is more difficult because complex solutions of the Riccati equation (1.4) may “blow up in finite time”. Nevertheless, we can hope to avoid singularities of the Riccati equation by choosing the initial condition $y(0)$ suitably.

In this paper, we focus on the analysis of solutions of the Riccati equation for specific initial conditions $y(0)$. This is justified because our estimates also give rise to corresponding estimates for general approximate Schrödinger wave functions, using the following procedure. Suppose that a specific y is known, up to a small error term. Then integrating (1.3), one obtains one fundamental solution $\phi_1(x) = \exp(\int^x y)$ of the Schrödinger equation. The other fundamental solution can readily be obtained by integrating the Wronskian equation $\phi_1' \phi_2 - \phi_1 \phi_2' = \text{const.}$ We thus obtain the general solution (1.2). Keeping track of the error in this procedure, one can derive error estimates for any Schrödinger wave function.

2. THE FLOW OF CIRCLES FOR A CONSTANT POTENTIAL

In this section we consider the special case of a constant potential. This case can easily be analyzed in closed form, and the resulting flow in the complex plane will be helpful for the geometric understanding of the invariant disk estimates. Thus assume that V is a non-zero complex constant. We set $\zeta = \sqrt{V}$. Then the general solution of the Schrödinger equation (1.1) is

$$\phi(x) = ae^{\zeta x} + be^{-\zeta x}, \quad x \in \mathbb{R}$$

with $a, b \in \mathbb{C}$. The corresponding solution of the Riccati equation is

$$\begin{aligned} y(x) &= \zeta \frac{ae^{\zeta x} - be^{-\zeta x}}{ae^{\zeta x} + be^{-\zeta x}} = \zeta \frac{(a-b) \cosh(\zeta x) + (a+b) \sinh(\zeta x)}{(a+b) \cosh(\zeta x) + (a-b) \sinh(\zeta x)} \\ &= \zeta \frac{(a-b) + \tau(x)(a+b)}{(a+b) + \tau(x)(a-b)}, \end{aligned}$$

where $\tau(x) := \tanh(\zeta x)$. Setting $y_0 = y(0)$,

$$y_0 = \zeta \frac{a-b}{a+b},$$

we can express y in terms of y_0 ,

$$y(x) = \zeta \frac{y_0 + \tau(x)\zeta}{\tau(x)y_0 + \zeta}.$$

Note that the mapping $y_0 \rightarrow y$ is a fractional linear transformation. It has the fixed points $y = \pm\zeta$ corresponding to the two solutions $\phi = e^{\pm\zeta x}$, respectively. Furthermore, we see that circles are mapped onto circles or straight lines. Thus by varying x , we obtain a flow of circles in the complex plane. To analyze this flow, let us assume that y_0 lies on a circle of radius R_0 around m_0 , i.e.

$$y_0 = m_0 + z \quad \text{with} \quad z = R_0 e^{i\varphi}.$$

Then for any fixed x ,

$$y = \zeta \frac{z + m_0 + \tau\zeta}{\tau z + \tau m_0 + \zeta}.$$

Thus for any $m \in \mathbb{C}$, we can write

$$y - m = \frac{(\zeta - \tau m)R_0 e^{i\varphi} + \zeta m_0 + \tau\zeta^2 - \tau m m_0 - m\zeta}{\tau R_0 e^{i\varphi} + \tau m_0 + \zeta} = \frac{c}{e^{i\varphi}} \left(\frac{e^{i\varphi} + \gamma}{e^{-i\varphi} + \delta} \right),$$

where the introduced quantities

$$c = \frac{(\zeta - \tau m)R_0}{\tau m_0 + \zeta}, \quad \gamma = \frac{\zeta m_0 + \tau\zeta^2 - \tau m m_0 - m\zeta}{(\zeta - \tau m)R_0}, \quad \delta = \frac{\tau R_0}{\tau m_0 + \zeta}$$

are independent of φ . For m to be the center of the new circle, the resulting expression for $|y-m|$ must be independent of φ . This gives the condition $\gamma = \bar{\delta}$. We thus conclude that

$$|y-m| = R,$$

where the center and radius are given by

$$m = \zeta \frac{(m_0 + \tau\zeta)(\overline{\tau m_0 + \zeta}) - R_0^2 \bar{\tau}}{|\tau m_0 + \zeta|^2 - R_0^2 |\tau|^2}, \quad R = \frac{R_0 |\tau^2 - 1| |\zeta|^2}{|\tau m_0 + \zeta|^2 - R_0^2 |\tau|^2}.$$

The denominator can have zeros, in which case the circle degenerates to a straight line. Whenever the denominator has no zeros, we can take the limit $x \rightarrow \infty$ to find that in the case $\operatorname{Re} \zeta > 0$, the circle asymptotically approaches the fixed point $y = \zeta$, unless if we start at $m_0 = -\zeta$ with $R_0 = 0$. Thus we can say that $y = \zeta$ is the stable and $y = -\zeta$ the unstable fixed point. Conversely, in the case $\operatorname{Re} \zeta < 0$, the fixed point $y = \zeta$ is unstable, whereas $y = -\zeta$ is stable. The flow of circles is illustrated in Figure 1 (left).

In the remaining case $\operatorname{Re} \zeta = 0$, we clarify the situation by computing the stationary circles. In this case, ζ and τ are purely imaginary, and thus the above formula for R becomes

$$R = R_0 \zeta^2 \frac{\tau^2 - 1}{\tau^2(R_0^2 - |m_0|^2) - 2\tau \zeta \operatorname{Re}(m_0) - \zeta^2}.$$

For a stationary circle, R must equal R_0 , for all imaginary τ (because the range of the function $\tanh(\zeta x)$ is $i\mathbb{R}$). Multiplying by the denominator, we get a quadratic polynomial in τ , and comparing the coefficients, we obtain the conditions

$$\operatorname{Re} m_0 = 0 \quad \text{and} \quad |m_0|^2 - R_0^2 = |\zeta|^2.$$

We thus obtain for any $R_0 \geq 0$ the two circles with centers

$$m_0 = \pm i \sqrt{R_0^2 + |\zeta|^2}, \quad (2.1)$$

and an easy computation shows that these circles are indeed stationary under the flow. Since these circles enclose the fixed points (see Figure 1 (right)), both fixed points are centers.

This simple analysis gives rise to a useful concept. Namely, the above flow of circles under the Riccati equation defines an invariant region consisting of the interior of the circles together with their boundary. In the next section we shall implement this point of view in the case of a non-constant potential V .

3. INVARIANT DISK ESTIMATES FOR THE RICCATI EQUATION

We now turn our attention to solutions $y \in \mathbb{C}$ of the Riccati equation (1.4) for a general complex-valued potential $V(x)$. Our goal is to derive inequalities of the form

$$|y(x) - m(x)| \leq R(x)$$

for explicit functions m and R . Geometrically, this means that the exact solution y stays inside the disk of radius R centered at m . Thus we can interpret m as an approximate solution, with R giving a rigorous bound on the error.

In preparation, we show that the flow given by the Riccati equation maps circles into circles. At the same time, we derive differential equations describing the motion of these circles. Let us assume that y lies on a circle of radius R centered at m , i.e.

$$y = m + R e^{i\varphi},$$

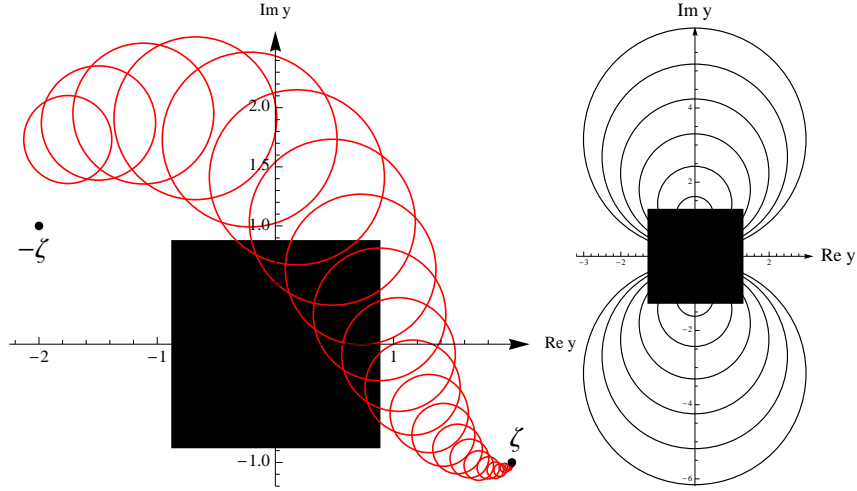


FIGURE 1. Example for flow of circles with $\zeta = 2 - i$ (left) and stationary circles in the case $\zeta = i$ (right).

where $R \geq 0$, $\varphi \in \mathbb{R}$, $m \in \mathbb{C}$. We now derive differential equations for R and m . First,

$$\begin{aligned} m' + R'e^{i\varphi} + i\varphi' Re^{i\varphi} &= y' \\ &= V - y^2 = V - m^2 - 2Rme^{i\varphi} - R^2e^{2i\varphi}. \end{aligned}$$

We multiply by $e^{-i\varphi}$ and take the real parts to get

$$\operatorname{Re} [e^{-i\varphi}(V - m^2 - m') - 2Rm - R' - i\varphi' R - e^{i\varphi} R^2] = 0.$$

In taking the real part, the term involving φ' drops out. Furthermore, we may replace the factor $e^{i\varphi}$ by $e^{-i\varphi}$. This gives

$$\operatorname{Re} [e^{-i\varphi}(V - m^2 - m' - R^2) - 2Rm - R'] = 0.$$

Since this equation should hold for any φ , we obtain the system of ODEs

$$\begin{aligned} R' &= -2R \operatorname{Re} m \\ m' &= V - m^2 - R^2. \end{aligned}$$

It is difficult to solve this system exactly. But the following lemma gives us a method to obtain invariant disk estimates.

Lemma 3.1. *For a given complex-valued potential $V = V(x)$, we assume that the complex function m and the real function $R \geq 0$ satisfy on the interval $I := [x_0, x_1]$ the differential equations*

$$R' = -2R \operatorname{Re} m + \delta R \tag{3.1}$$

$$m' = V - m^2 - R^2 + \delta m, \tag{3.2}$$

where the real function δR and the complex function δm obey the inequality

$$\delta R \geq |\delta m|. \tag{3.3}$$

Then the disk with radius R centered at m is invariant, i.e. for any solution of the Riccati equation (1.4) the following implication holds:

$$|y - m|(x_0) \leq R(x_0) \implies |y - m|(x) \leq R(x) \quad \forall x \in I.$$

Proof. We first prove the lemma in the case of strict inequality in (3.3). If the lemma were false, there would be an $x \in I$ such that $|y - m|(x) > R(x)$. Let $\bar{x} \in [x_0, x_1]$ be the infimum of all such x . Then $|y - m|(\bar{x}) = R(\bar{x})$. Using (1.4) and (3.2), we find at \bar{x}

$$\begin{aligned} \frac{d}{dx}|y - m| &= \operatorname{Re} \frac{(y' - m')\overline{(y - m)}}{|y - m|} = \operatorname{Re} \frac{(V - y^2 - V + m^2 + R^2 - \delta m)\overline{(y - m)}}{|y - m|} \\ &\leq R \operatorname{Re}(y - m) + |\delta m| - \operatorname{Re} \frac{(y^2 - m^2)\overline{(y - m)}}{|y - m|} \\ &= R \operatorname{Re}(y - m) + |\delta m| - R \operatorname{Re}(y + m) = -2R \operatorname{Re} m + |\delta m|. \end{aligned}$$

Combining this with (3.1) and the strict inequality in (3.3), we obtain

$$\frac{d}{dx}|y - m|(\bar{x}) < \frac{d}{dx}R(\bar{x}).$$

Hence there is a $\delta > 0$ such that on the interval $(\bar{x}, \bar{x} + \delta)$ the inequality $|y - m| < R$ holds. This is a contradiction.

To prove the general case of non-strict inequality in (3.3), we introduce the new radius \tilde{R} by

$$\tilde{R} = R + \varepsilon e^{L(x-x_1)},$$

where $\varepsilon > 0$ and

$$L > \max_I \left(-2 \operatorname{Re} m + 2R - \varepsilon e^{L(x-x_1)} \right). \quad (3.4)$$

Then \tilde{R} and m satisfy again the differential equations (3.1) and (3.2), where R is replaced by \tilde{R} , and δR and δm are replaced by

$$\begin{aligned} \delta \tilde{R} &= \delta R + \varepsilon e^{L(x-x_1)} (L + 2 \operatorname{Re} m) \\ \delta \tilde{m} &= \delta m + \varepsilon e^{L(x-x_1)} \left(2R - \varepsilon e^{L(x-x_1)} \right). \end{aligned}$$

Using (3.3) and (3.4), we see that $|\delta \tilde{m}| < \delta \tilde{R}$ for sufficiently small ε , and thus the circle with radius \tilde{R} and center m is invariant. Letting $\varepsilon \searrow 0$ completes the proof. \square

In what follows, it is convenient to write $m = \alpha + i\beta$ with real α and β , and similarly we write $\delta m = \delta\alpha + i\delta\beta$. Then the equations (3.1) and (3.2) become

$$R' = -2\alpha R + \delta R \quad (3.5)$$

$$\alpha' = \operatorname{Re} V - \alpha^2 + \beta^2 - R^2 + \delta\alpha \quad (3.6)$$

$$\beta' = \operatorname{Im} V - 2\alpha\beta + \delta\beta. \quad (3.7)$$

In our first theorem we satisfy the conditions of Lemma 3.1 by employing a special ansatz where the invariant disks are centered on the real axis (so that $\beta \equiv 0$). We introduce the abbreviation

$$\boxed{U = \operatorname{Re} V - \alpha^2 - \alpha'} \quad (3.8)$$

Theorem 3.2. *Suppose that on an interval $I \subset \mathbb{R}$, we are given the real functions $\alpha, W \in C^1(I)$. Assume furthermore that $W > 0$ and that*

$$2\alpha W + \frac{W'}{2} - \sqrt{W} \left(|W - U| + |\operatorname{Im} V| \right) \geq 0. \quad (3.9)$$

Then the circle with radius R centered at m with

$$R = \sqrt{W}, \quad m = \alpha \quad (3.10)$$

is invariant on I under the Riccati flow (1.4).

Proof. We shall verify the conditions of Lemma 3.1. Using the ansatz (3.10) in the equations (3.5), (3.6) and (3.7), we get

$$\delta R = \frac{W'}{2\sqrt{W}} + 2\alpha\sqrt{W}, \quad \delta\alpha = W - U, \quad \delta\beta = -\operatorname{Im} V.$$

The sufficient condition $\delta R \geq |\delta\alpha| + |\delta\beta|$ reduces to (3.9). \square

In our next theorem we will not prescribe β . For convenience, we now replace (3.3) by the sufficient condition

$$\delta R = |\delta\alpha| + |\delta\beta|. \quad (3.11)$$

Thus our task is to find six functions R , α , β , δR , $\delta\alpha$ and $\delta\beta$ which satisfy the equations (3.5), (3.6) and (3.7) together with the condition (3.11). Thus we expect that we can freely assign two functions, and then the remaining four functions will be determined. To explain which functions are to be preassigned, we note that the equations (3.5) and (3.7) are both linear, so that the only nonlinearity appears in the α -equation (3.6). Thus we can get rid of the nonlinear differential equation by taking the functions

$$\alpha \quad \text{and} \quad W := R^2 - \beta^2 \quad (3.12)$$

as a-priori given. Then (3.6) becomes the defining equation for $\delta\alpha$; namely,

$$\delta\alpha = -\operatorname{Re} V + \alpha^2 + \alpha' + W.$$

Using these definitions, we are left with the system of equations

$$R' = -2\alpha R + |\delta\alpha| + |\delta\beta| \quad (3.13)$$

$$\beta' = \operatorname{Im} V - 2\alpha\beta + \delta\beta \quad (3.14)$$

$$R^2 - \beta^2 = W \quad (3.15)$$

for the three unknown functions R , β and $\delta\beta$. This system consists of two linear differential equations and one nonlinear algebraic equation. Of course, we must also ensure that $0 \leq R < \infty$.

To analyze these equations, we consider the two cases $\delta\beta \geq 0$ and $\delta\beta < 0$ separately.

Case (A) $\delta\beta \geq 0$: Subtracting (3.14) from (3.13) we get

$$(R - \beta)' = -2\alpha(R - \beta) - \operatorname{Im} V + |\delta\alpha|. \quad (3.16)$$

Furthermore, differentiating (3.15) gives

$$2RR' - 2\beta\beta' = W'. \quad (3.17)$$

We consider (3.16) and (3.17) as a system of two linear algebraic equations in the unknowns R' and β' . Solving for β' and substituting into (3.14), we find

$$(R - \beta)\delta\beta = -R|\delta\alpha| + 2W\alpha + \operatorname{Im} V \beta + \frac{W'}{2}. \quad (3.18)$$

Since we assumed $\delta\beta$ to be positive, we get the consistency condition

$$(R - \beta) \left[2\alpha W + \frac{W'}{2} - R|\delta\alpha| + \beta \operatorname{Im} V \right] \geq 0. \quad (3.19)$$

Provided that this consistency condition holds, we can use (3.16) to solve for $R - \beta$. Then using (3.15), we conclude that $R + \beta = W/(R - \beta)$.

Case (B) $\delta\beta < 0$: Adding (3.13) and (3.14) gives

$$(R + \beta)' = -2\alpha(R + \beta) + \operatorname{Im} V + |\delta\alpha|. \quad (3.20)$$

Solving (3.20) and (3.17) for β' and substituting the result into (3.14), we obtain

$$(R + \beta)\delta\beta = R|\delta\alpha| - 2W\alpha - \operatorname{Im} V \beta - \frac{W'}{2},$$

giving rise in this case to the consistency condition

$$(R + \beta) \left[2\alpha W + \frac{W'}{2} - R|\delta\alpha| + \beta \operatorname{Im} V \right] \geq 0. \quad (3.21)$$

Provided that this consistency condition holds, $R + \beta$ is determined by (3.20), and $R - \beta = W/(R + \beta)$.

Since the bracket in (3.19) and (3.21) will appear often, it is convenient to introduce the abbreviation

$$\mathfrak{D} = 2\alpha W + \frac{W'}{2} - R|\delta\alpha| + \beta \operatorname{Im} V. \quad (3.22)$$

We refer to \mathfrak{D} as the **determinator**. Then the following invariant disk estimate holds.

Theorem 3.3. *Suppose that on an interval $I \subset \mathbb{R}$, we are given the real functions $\alpha, W \in C^1(I)$. We set*

$$\sigma(x) = \exp \left(\int^x 2\alpha \right). \quad (3.23)$$

Then the following statements hold.

(A) *Define real functions R and β on I by*

$$(R - \beta)(x) = \frac{1}{\sigma} \int^x \sigma (-\operatorname{Im} V + |W - U|) \quad (3.24)$$

$$(R + \beta)(x) = \frac{W(x)}{(R - \beta)(x)} \quad (3.25)$$

(with U as defined by (3.8)). Assume that the function $R - \beta$ has no zeros, $R \geq 0$, and that

$$(R - \beta) \mathfrak{D} \geq 0 \quad (3.26)$$

(with \mathfrak{D} according to (3.22)). Then the circle centered at $m(x) = \alpha + i\beta$ with radius $R(x)$ is invariant on I under the Riccati flow (1.4).

(B) *Define real functions R and β on I by*

$$(R + \beta)(x) = \frac{1}{\sigma} \int^x \sigma (\operatorname{Im} V + |W - U|) \quad (3.27)$$

$$(R - \beta)(x) = \frac{W(x)}{(R + \beta)(x)}. \quad (3.28)$$

Assume that the function $R + \beta$ has no zeros, $R \geq 0$, and that

$$(R + \beta) \mathfrak{D} \geq 0. \quad (3.29)$$

Then the circle centered at $m(x) = \alpha + i\beta$ with radius $R(x)$ is invariant on I under the Riccati flow (1.4).

Proof. We only prove the first part, as the proof of the second part is similar. Since (3.26) holds, we are consistently in Case (A) above. Integrating the differential equation (3.16) gives (3.24), whereas (3.25) follows from (3.12). We thus have a solution of the system of equations (3.13), (3.14) and (3.15) with $\delta\beta$ given by (3.18). Applying Lemma 3.1 completes the proof. \square

We next outline the general strategy for applying the last theorem. Suppose that an approximate solution \tilde{y} of the Riccati equation is given. Setting $\tilde{V} = \tilde{y}' + \tilde{y}^2$, we can consider \tilde{y} as a solution of a Riccati equation

$$\tilde{y}' = \tilde{V} - \tilde{y}^2 \quad (3.30)$$

with an “approximate” potential \tilde{V} . Since \tilde{y} approximates y , an obvious idea would be to consider circles centered at $m = \tilde{y}$. In the estimates of Theorem 3.3, however, we only need to prescribe the function $\alpha = \operatorname{Re} m$, whereas the imaginary part of m will then be determined. Therefore, it is natural to choose

$$\alpha = \operatorname{Re} \tilde{y}. \quad (3.31)$$

A natural choice for W is to set

$$W = U \quad (3.32)$$

(with U according to (3.8)), because then the term $|W - U|$ in (3.24) and (3.27) vanishes¹. Then Theorem 3.3 gives us invariant disk estimates. The center m of this disk can be viewed as an improved approximate solution, and its error, measured as the distance from the exact solution, is at most R . The invariant disk estimate depends crucially on the sign of the determinant \mathfrak{D} . Thus in applications it is important to know the sign of \mathfrak{D} . It can even be useful to modify \tilde{y} so as to give \mathfrak{D} a desired sign (this will be illustrated in Section 5 in a few examples). For this purpose, it is useful to bring the determinant into a more convenient form.

Lemma 3.4. *Suppose that, for a given solution \tilde{y} of an approximate Riccati equation (3.30), α and W are chosen according to (3.31) and (3.32). Then the determinant is given by*

$$\mathfrak{D} = 2\alpha \operatorname{Re}(V - \tilde{V}) + \frac{1}{2} \operatorname{Re}(V - \tilde{V})' - \tilde{\beta} \operatorname{Im} \tilde{V} + \beta \operatorname{Im} V, \quad (3.33)$$

where $\tilde{\beta} = \operatorname{Im} \tilde{y}$.

Proof. Writing the Riccati equation (3.30) as

$$\alpha' = \operatorname{Re} \tilde{V} - \alpha^2 + \tilde{\beta}^2, \quad \tilde{\beta}' = \operatorname{Im} \tilde{V} - 2\alpha\tilde{\beta},$$

we can use (3.32) and (3.8) to obtain

$$W = U = \operatorname{Re}(V - \tilde{V}) - \tilde{\beta}^2.$$

Applying these identities in (3.22) gives

$$\mathfrak{D} = 2\alpha \operatorname{Re}(V - \tilde{V}) + \frac{1}{2} \operatorname{Re}(V - \tilde{V})' - 2\alpha\tilde{\beta}^2 - \tilde{\beta}\tilde{\beta}' + \beta \operatorname{Im} V.$$

Using the $\tilde{\beta}'$ -equation finishes the proof. \square

¹Other choices of W might be useful, but we will not consider them in this paper.

4. ERROR ESTIMATES FOR REAL POTENTIALS AND EXAMPLES

In this section we shall illustrate our error estimates in examples for a real potential V and explain how the previous results from [3, 2] fit into our framework. We first mention an additional structural relation which appears only for a real potential. Namely, suppose that ϕ is a complex solution of the Schrödinger equation (1.1). Decomposing it into its real and imaginary parts, $\phi = \phi_1 + i\phi_2$, the functions ϕ_1 and ϕ_2 are real solutions of the Schrödinger equation forming a fundamental set. Thus their Wronskian $w = \phi_1\phi_2' - \phi_1'\phi_2$ is a constant. It can be expressed as $w = \text{Im}(\bar{\phi}\phi') = |\phi|^2 \text{Im } y$, giving rise to the relation

$$|\phi|^2 = \frac{w}{\text{Im } y},$$

which is useful for estimating the amplitude of ϕ . Moreover, this relation shows that the imaginary part of y can never change sign, and thus the upper and lower half planes must be invariant regions for y .

To illustrate how our estimates apply, we begin with a simple example.

Example 4.1. (negative, increasing potential) Suppose that the potential satisfies on the interval $I = [x_0, x_1]$ the conditions

$$V(x) \leq 0, \quad V'(x) \geq 0.$$

The simplest (but certainly not the best) choice is to set $\alpha \equiv 0$. Furthermore, setting $W = U$, we see from (3.23) that σ is a constant. According to (3.8), we find that $W = V$. The determinant (3.22) simplifies to

$$\mathfrak{D} = \frac{V'}{2} \geq 0. \quad (4.1)$$

We want to apply part (B) of Theorem 3.3 (part (A) is similar if one flips the sign of β). From (3.27) we see that $R + \beta$ is a constant, which according to (3.29) and (4.1) must be positive. We thus obtain

$$\beta + R = c > 0, \quad \beta - R = \frac{|V|}{c}. \quad (4.2)$$

The condition $R \geq 0$ gives the constraint

$$c^2 \geq \max_I |V| = |V(x_0)|.$$

If the potential is constant, we recover the stationary circles of Section 2 (as is easily verified by comparing (4.2) and (2.1)). If the potential is non-constant, we get an increasing family of invariant disks in the upper half plane centered on the imaginary axis whose highest point is fixed at ic , and whose lowest point varies like $i|V|/c$; see Figure 2. \diamond

We next consider the situation for a general real potential V and a general choice of α , again setting $W = U$. Then the determinant becomes

$$\mathfrak{D} = 2\alpha U + \frac{U'}{2} = \frac{U}{2} \frac{(\sigma^2 U)'}{\sigma^2 U} \quad (4.3)$$

(with σ defined by (3.23)). The main simplification is that now \mathfrak{D} is an a-priori given function. In the case when $R - \beta$ and $R + \beta$ have opposite signs, we see from (3.26) and (3.29) that, depending on the sign of \mathfrak{D} , either part (A) or part (B) of Theorem 3.3 applies. In this case, we can combine parts (A) and (B) to obtain a statement which can be used even if \mathfrak{D} changes sign infinitely often. In view of (3.15), the condition

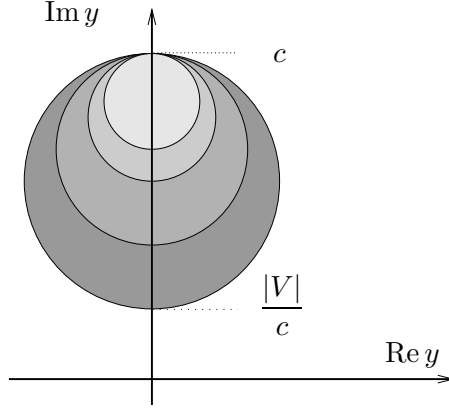


FIGURE 2. A simple invariant disk estimate for a negative, increasing potential.

that $R - \beta$ and $R + \beta$ should have opposite signs is equivalent to the simpler condition that $U < 0$; it means that the invariant disk either lies in the upper half plane or in the lower half plane, without intersecting the real line. By continuity, the invariant disk cannot move from the upper to the lower half plane. Thus we can assume without loss of generality that the invariant disk lies in the upper half plane. This means that $R + \beta > 0$ and $R - \beta < 0$. It is convenient to satisfy the equation (3.15) (and thus also (3.25) and (3.28)) by making the ansatz

$$\beta = \frac{\sqrt{|U|}}{2} \left(T + \frac{1}{T} \right), \quad R = \frac{\sqrt{|U|}}{2} \left(T - \frac{1}{T} \right) \quad (4.4)$$

with a free function $T > 1$. If \mathfrak{D} is negative, we apply Theorem 3.3 (A) to obtain

$$T = -\frac{\sqrt{|U|}}{R - \beta} = -\frac{\sigma \sqrt{|U|}}{c}$$

with c an integration constant. Differentiating gives

$$\frac{T'}{T} = \frac{(\sigma \sqrt{|U|})'}{\sigma \sqrt{|U|}} = \frac{1}{2} \frac{(\sigma^2 |U|)'}{\sigma^2 |U|} = \frac{1}{2} \frac{(\sigma^2 U)'}{\sigma^2 U} = \frac{1}{2} \left| \frac{(\sigma^2 U)'}{\sigma^2 U} \right|,$$

where in the last two steps we used that U is negative, and that in the considered case $\mathfrak{D} < 0$, the term $(\sigma^2 U)' / (\sigma^2 U)$ is positive according to (4.3). If \mathfrak{D} is positive, we apply Theorem 3.3 (B) to get

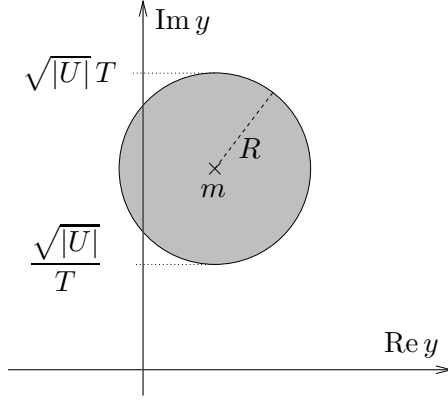
$$T = \frac{R + \beta}{\sqrt{|U|}} = \frac{c}{\sigma \sqrt{|U|}}.$$

Now differentiating gives

$$\frac{T'}{T} = -\frac{(\sigma \sqrt{|U|})'}{\sigma \sqrt{|U|}} = -\frac{1}{2} \frac{(\sigma^2 U)'}{\sigma^2 U} = \frac{1}{2} \left| \frac{(\sigma^2 U)'}{\sigma^2 U} \right|,$$

where in the last step we used that now $(\sigma^2 U)' / (\sigma^2 U) < 0$. We conclude that, independent of the sign of \mathfrak{D} , we obtain the differential equation

$$\frac{T'}{T} = \frac{1}{2} \left| \frac{(\sigma^2 U)'}{\sigma^2 U} \right|.$$

FIGURE 3. Invariant disk estimate for $U < 0$.

Integrating both sides, we can rewrite T as a total variation,

$$T(x) = T_0 \exp \left(\frac{1}{2} \text{TV}_{[x_0, x]} \log |\sigma^2 U| \right). \quad (4.5)$$

In this way, we recover the invariant disk estimate which was first obtained in [3, Lemma 4.1]; see Figure 3.

Lemma 4.2. *Let α be a real function on $[x_0, x_1]$ which is continuous and piecewise C^1 . Suppose that the function $U := V - \alpha^2 - \alpha'$ is negative on $[x_0, x_1]$. Using the above definitions (4.5) and (4.4), the disks of radius R centered at $m = \alpha + i\beta$ are invariant under the Riccati flow (1.4), on $[x_0, x_1]$.*

We now illustrate in two examples how this lemma can be applied (for other applications see [3, Theorems 4.2 and 4.3] and [2, Lemmas 4.10 and 4.12]). In the first example, we consider the case that the potential V is negative. We recall that the WKB wave functions are given by (see for example [9, Section 2.4] or [5])

$$\phi_{\text{WKB}}(x) = |V(x)|^{-\frac{1}{4}} \exp \left(\pm i \int^x \sqrt{|V|} \right). \quad (4.6)$$

A short calculation shows that these functions satisfy the equation

$$\frac{d^2}{dx^2} \phi_{\text{WKB}} - V \phi_{\text{WKB}} = \left(\frac{5}{16} \frac{|V|^{\prime 2}}{|V|^2} - \frac{1}{4} \frac{|V|''}{|V|} \right) \phi_{\text{WKB}}.$$

Interpreting the right side as an error term, one sees that the WKB wave functions are expected to be a good approximation to ϕ provided that

$$\left| \frac{V''}{V^2} \right| + \left| \frac{V'^2}{V^3} \right| \ll 1. \quad (4.7)$$

For definiteness, we consider the plus sign in (4.6) (the minus sign can be obtained by complex conjugation). Then the corresponding approximate Riccati solution is given by

$$y_{\text{WKB}} = \frac{\phi'_{\text{WKB}}}{\phi_{\text{WKB}}} = i\sqrt{|V|} - \frac{V'}{4V}.$$

Following the general strategy described after Theorem 3.3, we thus choose

$$\alpha = \operatorname{Re} y_{\text{WKB}} = -\frac{V'}{4V}. \quad (4.8)$$

An easy computation gives

$$\alpha' = -\frac{V''}{4V} + \frac{V'^2}{4V^2} \quad (4.9)$$

$$U = V \left(1 + \frac{V''}{4V^2} + \frac{5V'^2}{16|V|^3} \right) \quad (4.10)$$

$$\sigma = \exp \left(-\frac{1}{2} \int^x \frac{V'}{V} \right) = \frac{c}{\sqrt{|V|}} \quad (4.11)$$

$$\sigma^2 U = -c^2 \left(1 + \frac{V''}{4V^2} + \frac{5V'^2}{16|V|^3} \right). \quad (4.12)$$

In view of (4.10), the condition (4.7) and the fact that $V < 0$, we see that U is negative. Thus Lemma 4.2 applies, giving the following estimate.

Example 4.3. (error estimate for WKB wave function, $V < 0$)

Suppose that V is negative and

$$-\frac{V''}{4V^2} - \frac{5V'^2}{16|V|^3} < 1.$$

Then the disks of radius R centered at $m = \alpha + i\beta$ as given by (4.8), (4.4) and

$$T(x) = T_0 \exp \left(\frac{1}{2} TV_{[x_0, x]} \log \left[1 + \frac{V''}{4V^2} + \frac{5V'^2}{16|V|^3} \right] \right) \quad (4.13)$$

are invariant under the Riccati flow (1.4), on $[x_0, x_1]$.

In our setting, the semiclassical limit can be described by scaling the potential according to $V \rightarrow \lambda V$ and considering the behavior as $\lambda \rightarrow \infty$. In this limit, the square bracket in (4.13) converges to one, so that the logarithm vanishes. As a consequence, T becomes a constant. Choosing $T_0 = 1$, we find that the radius $R(x)$ as given by (4.4) vanishes identically in the semiclassical limit, in agreement with the fact that the WKB wave function goes over to the exact solution.

The next estimate even applies near a zero of the potential.

Example 4.4. (invariant disk estimate with exponential bound)

Choose a constant α ,

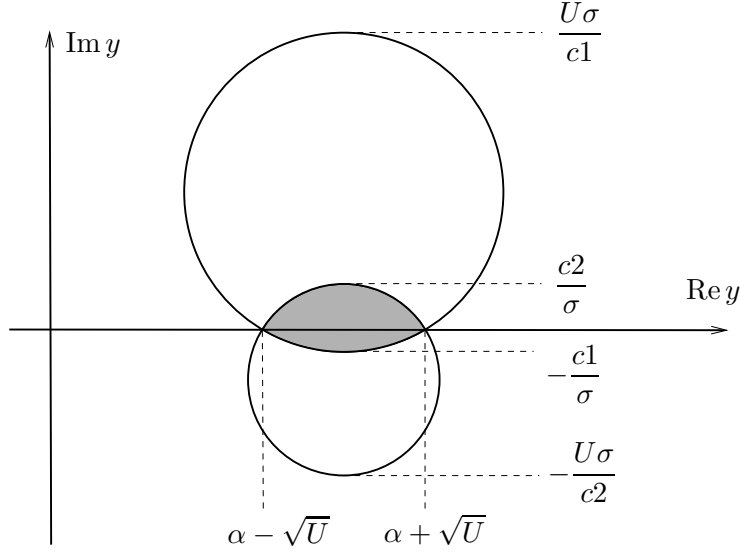
$$\alpha = c + \sup_{x \in [x_0, x_1]} \sqrt{\max(0, V(x))} \quad (4.14)$$

with $c \geq 0$. Then

$$\begin{aligned} U &= V - \alpha^2 < -c^2 \leq 0 \\ \sigma &= C e^{2\alpha x} \\ \sigma^2 U &= C^2 e^{4\alpha x} (V - \alpha^2) \end{aligned}$$

with an integration constant C . Hence Lemma 4.2 yields that the disks of radius R centered at $m = \alpha + i\beta$ as given by (4.14), (4.4) and

$$T(x) = T_0 \exp \left(\frac{1}{2} TV_{[x_0, x]} \log [e^{4\alpha x} (V - \alpha^2)] \right)$$

FIGURE 4. Invariant lens-shaped region estimate for $U > 0$.

are invariant under the Riccati flow (1.4), on $[x_0, x_1]$.

Clearly, due to the exponential factor $e^{4\alpha x}$, this estimate gets weaker as the size of the interval increases. We shall below see a much better estimate using Airy functions (see Example 5.1).

We next consider how Theorem 3.3 applies in the case $U \geq 0$ (where we again choose $W = U$). Then, according to (3.15), the functions $R - \beta$ and $R + \beta$ have the same sign, which must be positive because $R \geq 0$. Inspection of (3.26) and (3.29) yields that the determinant must be positive, i.e.

$$U' + 4\alpha U \geq 0. \quad (4.15)$$

Provided that this condition holds, we may apply both parts (A) and (B) of Theorem 3.3. Taking the intersection of the corresponding invariant disks gives the following result, which generalizes [2, Lemma 4.2].

Lemma 4.5. *Let α be a real function on $[x_0, x_1]$ which is continuous and piecewise C^1 . Suppose that the function $U := V - \alpha^2 - \alpha'$ is positive on $[x_0, x_1]$ and that the condition (4.15) holds. For any positive constants c_k , $k = 1, 2$, we introduce the two disks of radii R_k centered at $m_k = \alpha + i\beta_k$ with*

$$\begin{aligned} R_1 &= \frac{1}{2} \left(\frac{U\sigma}{c_1} + \frac{c_1}{\sigma} \right), & \beta_1 &= \frac{1}{2} \left(\frac{U\sigma}{c_1} - \frac{c_1}{\sigma} \right) \\ R_2 &= \frac{1}{2} \left(\frac{U\sigma}{c_2} + \frac{c_2}{\sigma} \right), & \beta_2 &= -\frac{1}{2} \left(\frac{U\sigma}{c_2} - \frac{c_2}{\sigma} \right). \end{aligned}$$

Then the two disks as well as the lens-shaped region obtained as their intersection are invariant under the Riccati flow (1.4).

As is easily verified, the boundaries of both disks intersect the real axis at the points $\alpha \pm \sqrt{U}$, and thus their intersection is non-void; see Figure 4.

In our next example we shall apply Lemma 4.5 to the WKB wave function for a positive potential. We thus assume that $V > 0$ and that (4.7) is again satisfied. Considering the WKB wave function

$$\phi_{\text{WKB}}(x) = V(x)^{-\frac{1}{4}} \exp\left(\int^x \sqrt{V}\right), \quad (4.16)$$

an easy computation shows that

$$\begin{aligned} y_{\text{WKB}}(x) &= \frac{\phi'_{\text{WKB}}}{\phi_{\text{WKB}}} = \sqrt{V} - \frac{V'}{4V} \\ \alpha &= \operatorname{Re} y_{\text{WKB}}(x) = \sqrt{V} - \frac{V'}{4V} \\ U &= V - \alpha^2 - \alpha' = -\frac{5}{16} \frac{V'^2}{V^2} + \frac{V''}{4V}. \end{aligned}$$

Unfortunately, in contrast to our previous example (4.10), now U need not have a fixed sign, and thus one cannot apply the above lemmas. Our method for getting around this problem is to consider in the WKB ansatz another potential V_{WKB} , and to set

$$\phi_{\text{WKB}}(x) = V_{\text{WKB}}(x)^{-\frac{1}{4}} \exp\left(\int^x \sqrt{V_{\text{WKB}}}\right).$$

Then

$$\alpha = \operatorname{Re} \frac{\phi'_{\text{WKB}}}{\phi_{\text{WKB}}} = \sqrt{V_{\text{WKB}}} - \frac{V'_{\text{WKB}}}{4V_{\text{WKB}}} \quad (4.17)$$

$$U = V - \alpha^2 - \alpha' = V - V_{\text{WKB}} - \frac{5}{16} \frac{V_{\text{WKB}}'^2}{V_{\text{WKB}}^2} + \frac{V_{\text{WKB}}''}{4V_{\text{WKB}}}. \quad (4.18)$$

By arranging that U has a definite sign, we may apply either Lemma 4.2 or Lemma 4.5. To give a simple example, we choose

$$V_{\text{WKB}} = \frac{V}{4}.$$

Then U is positive because V is positive and (4.7) holds. Furthermore, a direct computation gives

$$\sigma = \exp\left(\int^x 2\alpha\right) = \frac{1}{\sqrt{V}} \exp\left(\int^x \sqrt{V}\right) \quad (4.19)$$

$$\frac{2}{V} U = \frac{3}{2} + \left[-\frac{5}{8} \frac{V'^2}{V^3} + \frac{V''}{2V^2}\right] \quad (4.20)$$

$$\frac{2}{3V^{\frac{3}{2}}} (U' + 4\alpha U) = 1 + \left[-\frac{5}{12} \frac{V'^2}{V^3} + \frac{5}{8} \frac{V'^3}{V^{\frac{9}{2}}} + \frac{V''}{3V^2} - \frac{3V'V''}{4V^{\frac{7}{2}}} + \frac{V'''}{6V^{\frac{5}{2}}}\right]. \quad (4.21)$$

We are now in a position to apply Theorem 3.3.

Example 4.6. (error estimate for WKB wave function, $V > 0$)

Suppose that V is positive and that the square brackets in (4.20) and (4.21) are both greater than minus one. Then choosing U and σ according to (4.20) and (4.19), the lens-shaped region from Lemma 4.5 (see Figure 4) is invariant under the Riccati flow (1.4), on $[x_0, x_1]$.

It is worth noting that from (4.19), we see that σ grows exponentially. Hence the lens-shaped region gets thinner, improving the estimate exponentially fast.

The previous estimates using Lemma 4.2 and Lemma 4.5 have the disadvantage that if U changes sign, different kinds of estimates must be pasted together. This makes it necessary to match invariant disks (see [2, Lemma 4.4]). In the next section we explain a more convenient method in the more general context of a complex potential (but also working for real potentials) which makes it possible for the invariant disks to flow continuously across the real line.

5. ERROR ESTIMATES FOR APPROXIMATE WKB/AIRY SOLUTIONS FOR REAL OR COMPLEX POTENTIALS

In this section we illustrate the general technique for applying Theorem 3.2 and Theorem 3.3 by discussing typical examples. Based on Theorems 3.2 and 3.3, we will derive *rigorous error estimates* for the standard approximate solutions obtained by glueing together WKB and Airy wave functions.

For a given potential (real or complex), one can usually distinguish regions where $|V|$ is large, so that the solutions of the Schrödinger equation are well-approximated by WKB wave functions. In the remaining regions, one can approximate the potential by a linear potential, so that the Schrödinger equation can be solved explicitly in terms of Airy functions. To be more flexible, in the WKB region we consider the approximate solutions

$$\phi_{\text{WKB}}(x) = V_{\text{WKB}}(x)^{-\frac{1}{4}} \exp\left(\int^x \pm \sqrt{V_{\text{WKB}}} \right) \quad (5.1)$$

with a potential $V_{\text{WKB}} \approx V$, which will be determined later. Likewise, in the Airy region, our approximate wave functions are solutions of the Schrödinger equation

$$\phi_{\text{A}}''(x) = V_{\text{A}} \phi_{\text{A}}, \quad (5.2)$$

where $V_{\text{A}} \approx V$ is a linear function, also to be determined later. By the standard C^1 -glueing of the WKB and Airy functions, we obtain an approximate wave function $\tilde{\phi}$. The wave function $\tilde{\phi}$ is a weak solution of a Schrödinger equation

$$\tilde{\phi}'' = \tilde{V} \tilde{\phi}, \quad (5.3)$$

where \tilde{V} in the Airy region coincides with V_{A} , whereas in the WKB region a short calculation gives

$$\tilde{V} = V_{\text{WKB}} + \frac{5}{16} \frac{V_{\text{WKB}}^2}{V_{\text{WKB}}^2} - \frac{V_{\text{WKB}}''}{4V_{\text{WKB}}}. \quad (5.4)$$

Note that \tilde{V} is piecewise smooth, but in general has discontinuities. Following the strategy explained after Theorem 3.3, we introduce the function $\tilde{y} = \tilde{\phi}'/\tilde{\phi}$, which is continuous and piecewise smooth, satisfying the Riccati equation

$$\tilde{y}' = \tilde{V} - \tilde{y}^2. \quad (5.5)$$

We again introduce the (continuous, but only piecewise smooth) function α by

$$\alpha = \text{Re } \tilde{y}, \quad (5.6)$$

define U by (3.8) and (again for simplicity) choose $W = U$. We choose starting values for the functions β and R which are compatible with (3.15). We can then apply Theorem 3.3 in various ways. If $U < 0$, i.e. $R + \beta$ and $R - \beta$ have opposite signs, depending on the sign of the determinant \mathfrak{D} , we can apply either part (A)

or part (B). If however $U \geq 0$, the functions $R + \beta$ and $R - \beta$ are both positive, and thus Theorem 3.3 applies only if \mathfrak{D} is positive, and in this case we can apply both part (A) and part (B). If β becomes zero, it may be preferable to switch to the simpler estimate of Theorem 3.2, provided that the inequality (3.9) holds. In this way, we have different possibilities to obtain invariant disk estimates, and by taking their intersection one gets even sharper estimates involving lens-shaped invariant regions. Observe that on the boundaries between the WKB and Airy regions, the functions V and α' , and consequently also U , may have discontinuities. In order to satisfy (3.15), either $R + \beta$ or $R - \beta$ must “jump” discontinuously, in such a way that the new disk contains the old one.

The crucial point for making this procedure work is that one must be able to prescribe the sign of \mathfrak{D} or to satisfy the inequality (3.9). One method to achieve this is to modify the potentials V_{WKB} and V_A in (5.1) and (5.2). The effect on \mathfrak{D} of modifying the potentials can be seen most easily from Lemma 3.4. More specifically, in the WKB region, the term $2\alpha \operatorname{Re}(V - \tilde{V})$ in (3.33) can be suitably changed by modifying the real part of V_{WKB} , whereas the imaginary part of V_{WKB} affects the term $-\tilde{\beta} \operatorname{Im} \tilde{V}$. Note that the derivative term in (3.33) as well as the derivative terms in (5.4) only give rise to small corrections. In the Airy region, on the other hand, we can change the coefficients in the linear function $V_A(x)$ to modify the suitable terms in (3.33). In order to satisfy the condition (3.9), it may be useful to apply the identity

$$(3.9) = 2\alpha \operatorname{Re}(V - \tilde{V}) + \frac{1}{2} \operatorname{Re}(V - \tilde{V})' - \tilde{\beta} \operatorname{Im} \tilde{V} - |\operatorname{Im} V| \sqrt{\operatorname{Re}(V - \tilde{V}) - \tilde{\beta}^2}$$

(keeping in mind that in this case, $\beta \equiv 0$, and thus $\tilde{\beta}$ should be small), or else one can modify α , without respecting the relation (5.6).

We now give two concrete examples to illustrate this method. In the first example, the imaginary part of the potential is so small that the method works just as well for a real potential.

Example 5.1. We consider the potential (inspired by the spheroidal wave operator [3])

$$V = 10000 \left(-\frac{1}{2} + (1 + 0.05i) \sin^2 x \right), \quad (5.7)$$

on the interval $[0, \frac{\pi}{2}]$. Due to the large prefactor, the WKB condition (4.7) is satisfied except in a small neighborhood of the point $x = \frac{\pi}{4}$, where $|V|$ is small. Thus we divide our interval into three regions:

- (a) The “classically allowed” WKB region $[0, 0.715]$
- (b) The Airy region $[0.715, 0.83]$ near the “classical turning point”
- (c) The “classically forbidden” WKB region $[0.83, \frac{\pi}{2}]$

(The precise choice of the boundary points is arbitrary and has no major effect. Moreover, since the factor 0.05 is so small, we simply adopted the terminology from quantum mechanics, disregarding the effect of the imaginary part of the potential.) In the Airy region we approximate the potential by its linear Taylor series around the point $x = \frac{\pi}{4}$. We glue together the corresponding WKB and Airy functions, starting at $x = 0$ with the WKB wave function (5.1) with $V_{\text{WKB}} = V$ and choosing the plus sign. In the region (c) we also choose $V_{\text{WKB}} = V$. This gives the approximate wave function $\tilde{\phi}$, and we define the corresponding approximate Riccati solution by $\tilde{y} = \tilde{\phi}'/\tilde{\phi}$. Following the general procedure described earlier in this section, we choose α according to (5.6) and set $W = U$. To better illustrate our estimates, we choose the radius R of the

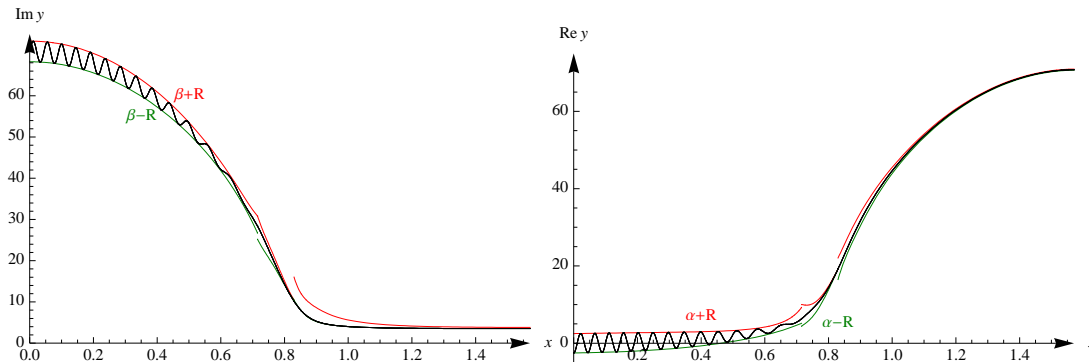


FIGURE 5. Upper and lower bounds for the imaginary (left) and real (right) parts of the Riccati solution in Example 5.1.

initial disk to be 2.5, although choosing it equal to zero would give a better estimate. In Figure 5 (left), the imaginary part of an exact numerical solution y starting on the boundary of the initial circle is plotted together with the upper bound $\beta + R$ and the lower bound $\beta - R$. Likewise, in Figure 5 (right), the real part of the solution as well as the upper bound $\alpha + R$ and the lower bound $\alpha - R$ are given. One sees that the invariant disks jump discontinuously at the glueing points, such that the new disk contains the old disk. In Figure 6,

the invariant disks are plotted for discrete values of x , and the black dots denote the exact solution at these values of x . We point out that the invariant disk always stays in the upper half plane. In region (c), the determinant is negative, so that part (A) of Theorem 3.3 applies. This means geometrically that the lower bound $\beta - R$ approaches the exact solution exponentially fast, whereas the upper bound $\beta + R$ is not as good an approximation.

In order to get a better upper bound, we changed the WKB potential in region (c) to

$$V_{\text{WKB}} = 0.9 V. \quad (5.8)$$

This makes the determinant negative, so that part (B) of Theorem 3.3 applies. Since V_{WKB} in (5.8) deviates considerably from V , we cannot expect that our approximation will be good in region (c). This is reflected in Figure 7 by the fact that R becomes large if x approaches $\frac{\pi}{2}$. Nevertheless, this estimate is still useful because the upper bound $\beta + R$ approaches the exact solution exponentially fast. Taking the intersection of the invariant disks with those from Figure 6, one gets lens-shaped invariant regions, thus estimating the exact solution up to exponentially decaying errors (see Figure 8). This exponential shrinkage of the invariant region can be understood by the fact that the potential is slowly varying, and that for a constant potential the solutions would tend exponentially fast to the stable fixed point \sqrt{V} (see Section 2).

Finally, in Figure 9 we show invariant disk estimates, where in region (c) we applied Theorem 3.2 and chose $\beta \equiv 0$. This estimate is not as good as the previous estimate, but on the other hand Theorem 3.2 is easier to apply, and the coarser estimate might be sufficient for some applications. \diamond

In the previous example, the semi-classical approximation was very good because of the large prefactor in (5.7). In our next example, the WKB/Airy wave function is not such a good approximation, making the error estimates more subtle. Moreover,

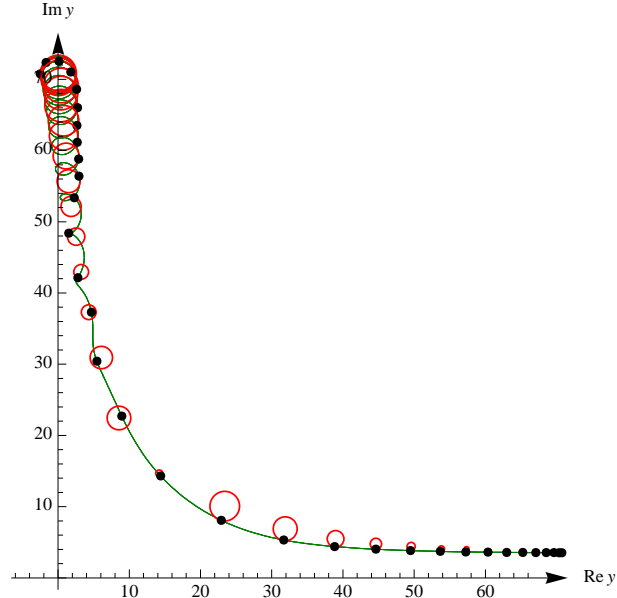


FIGURE 6. Invariant disks for the Riccati solution in Example 5.1.

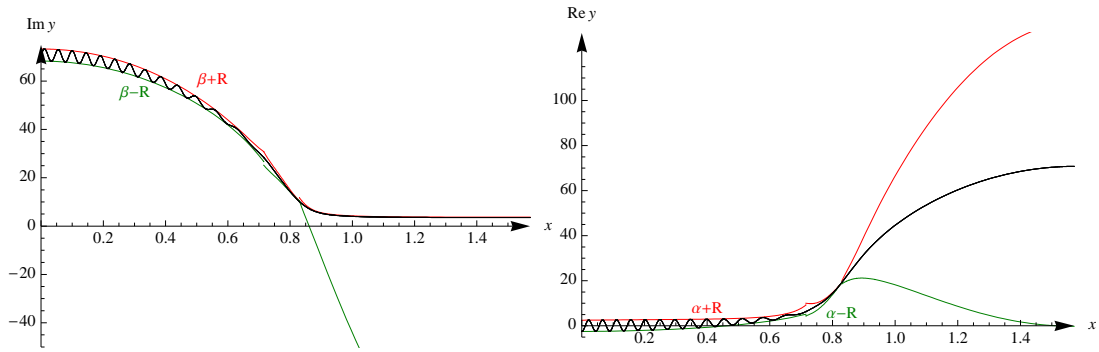
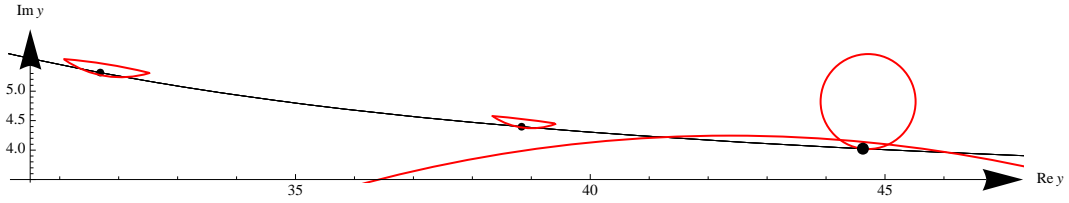
FIGURE 7. Upper and lower bounds after flipping the sign of \mathfrak{D} in Example 5.1.

FIGURE 8. Lens-shaped region estimates for the Riccati equation in Example 5.1.

the imaginary part of V has the opposite sign, thereby forcing the Riccati solution to cross the real axis. By suitably adjusting the sign of the determinant, we will arrange that the invariant disks also move from one half plane to the other.

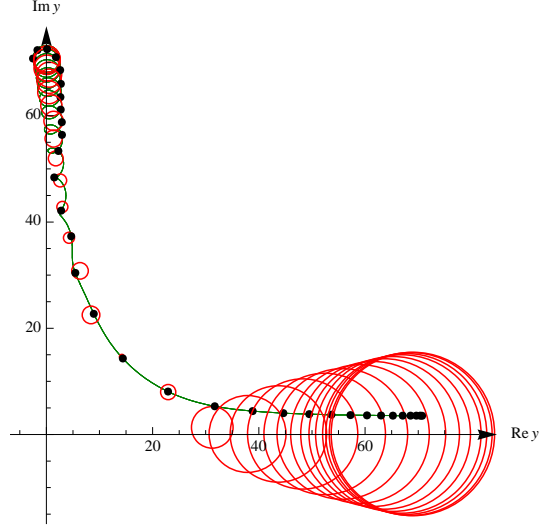


FIGURE 9. Invariant disk estimate applying Theorem 3.2 in Example 5.1.

Example 5.2. We consider on the interval $[0, \frac{\pi}{2}]$ the potential

$$V = 500 \left(-\frac{1}{2} + (1 - 0.2i) \sin^2 x \right).$$

We choose the WKB regions to be $[0, 0.52]$ (region (a)) and $[0.83, \frac{\pi}{2}]$ (region (c)), and the intermediate region $[0.52, 0.83]$ (region (b)) is the Airy region. In Figures 10 and 11 upper and lower bounds are given. In Figure 12 we plot the corresponding invariant disk estimates as well as lens-shaped invariant regions obtained by taking the intersection of the disks of Figures 10 and 11.

Note that now the invariant disks cross the real axis. When this happens, one must ensure when applying Theorem 3.3 that the denominator in (3.25) or (3.28) never becomes zero, because otherwise we would lose control of the estimates. This means that if the function $R - \beta$ vanishes, we must arrange the sign of the determinant such that case (A) applies, whereas $R + \beta$ may vanish only when we are in case (B). To this end, the potentials V_{WKB} and V_{A} are chosen as follows:

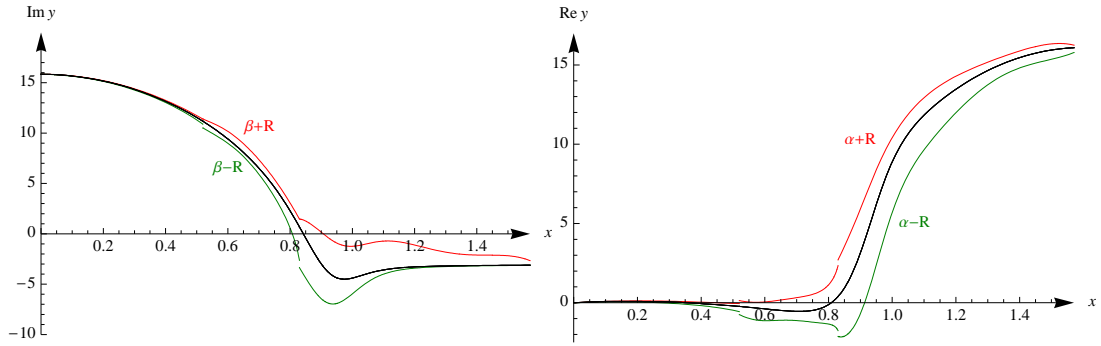


FIGURE 10. Upper and lower bounds for the imaginary (left) and real (right) parts of the Riccati solution in Example 5.2.

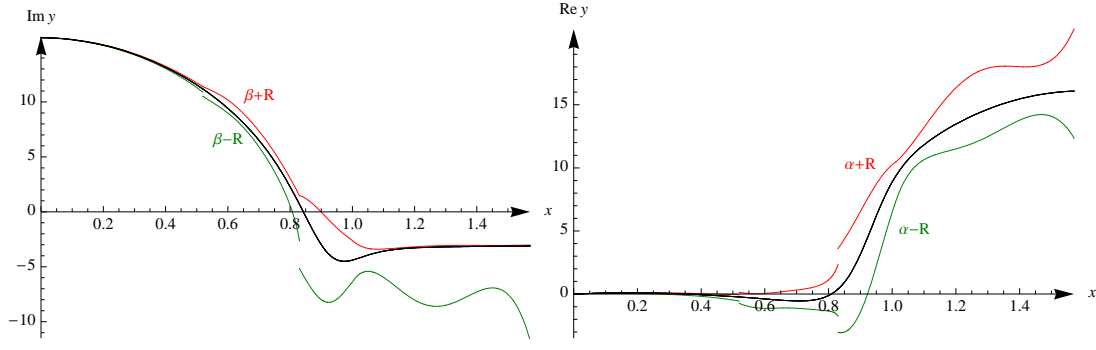
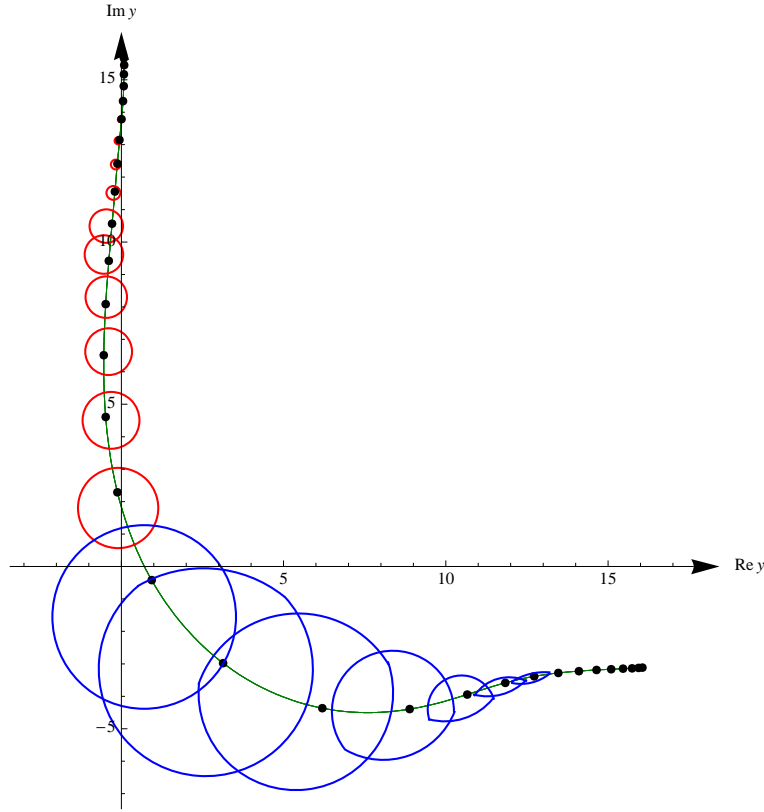
FIGURE 11. Upper and lower bounds after flipping the sign of \mathfrak{D} in Example 5.2.

FIGURE 12. Invariant disk (red) and lens-shaped region estimates (blue) for the Riccati equation in Example 5.2.

In region (a), we choose $V_{\text{WKB}} = V$. In region (b), for V_A we took the linear Taylor polynomial and decreased the real part of the linear term so as to make \mathfrak{D} positive. Then we are in case (B) of Theorem 3.3, in which the function $\beta - R$ can cross smoothly across the real line. Shortly after $\beta - R$ has become negative, we switch to case (A) of Theorem 3.3, so that $\beta + R$ can smoothly flip sign. For the estimates of Figure 10 we choose the potential $V_{\text{WKB}} = V$ in region (c) such that \mathfrak{D} is always positive. Then $\beta - R$ is a good approximation. For the estimates of Figure 11, however, we modified V_{WKB}

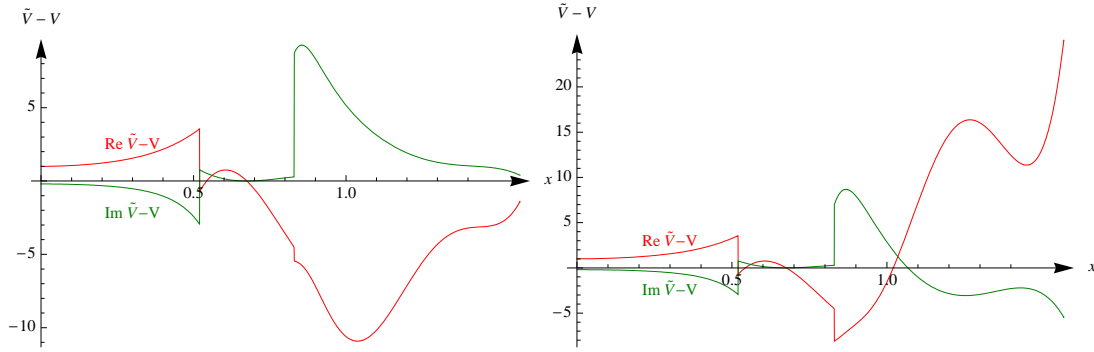


FIGURE 13. The potential $\tilde{V} - V$ as used for the estimates in Figure 10 (left) and Figure 11 (right).

in region (c) such as to arrange that \mathfrak{D} becomes negative, with the result that $\beta + R$ is a good approximation.

Our choice of the approximate potentials is shown in Figure 13, where we plot the real and imaginary parts of $\tilde{V} - V$, with \tilde{V} as in (5.3) and (5.5). We point out that the scale in these plots is one order of magnitude smaller than the scale of $V \sim 250$. This illustrates that slight modifications of the approximate potentials suffice to arrange the appropriate sign of \mathfrak{D} . The detailed form of the choice of the approximate potentials affects the function $\beta + R$ in Figure 10 (left) or the function $\beta - R$ in Figure 11 (left), as well as the functions $\alpha \pm R$ on the right of these figures. However, the corresponding lens-shaped invariant regions are insensitive to the detailed choice of \tilde{V} ; see Figure 12. \diamond

Acknowledgments: We would like to thank the referees for valuable comments. We are grateful to the Alexander-von-Humboldt Foundation as well as the Vielberth Foundation, Regensburg, for their generous support.

REFERENCES

- [1] B. Carter, “Black hole equilibrium states,” in *Black holes/Les astres occlus*, Ecole d’été Phys. Théor., Les Houches (1972)
- [2] F. Finster, N. Kamran, J. Smoller and S.-T. Yau, “Decay of solutions of the wave equation in the Kerr geometry,” gr-qc/0504047, *Commun. Math. Phys.* **264** (2006) 465-503
- [3] F. Finster, H. Schmid, “Spectral estimates and non-selfadjoint perturbations of spheroidal wave operators,” math-ph/0405010, *J. Reine Angew. Math.* **601** (2006) 71-107
- [4] S. Fraga, J.M. García de la Vega, E.S. Fraga, “The Schrödinger and Riccati Equations,” *Lecture Notes in Chemistry* **70**, Springer Verlag (1999)
- [5] N. Fröman, P.O. Fröman, “JWKB Approximation, Contributions to the Theory,” *North-Holland Publishing Company*, Amsterdam (1965)
- [6] G. Jona-Lasinio, F. Martinelli, E. Scoppola, “New approach to the semiclassical limit of quantum mechanics. I. Multiple tunnelings in one dimension,” *Commun. Math. Phys.* **80** (1981) 223-254
- [7] V.P. Maslov, M.V. Fedoriuk, “Semiclassical Analysis in Quantum Mechanics,” *Reidel*, Dordrecht (1981)
- [8] F.H. Molzahn, “A quantum WKB approximation without classical trajectories,” *J. Math. Phys.* **29** (1988) 2256-2267
- [9] J.J. Sakurai, “Modern Quantum Mechanics,” *Addison-Wesley Publishing Company* (1985)
- [10] S. Teukolsky, W.H. Press, “Perturbations of a rotating black hole. III. Interaction of the hole with gravitational and electromagnetic radiation,” *Astrophys. J.* **193** (1974), 443-461.

NWF I - MATHEMATIK, UNIVERSITÄT REGENSBURG, D-93040 REGENSBURG, GERMANY
E-mail address: `Felix.Finster@mathematik.uni-regensburg.de`

MATHEMATICS DEPARTMENT, THE UNIVERSITY OF MICHIGAN, ANN ARBOR, MI 48109, USA
E-mail address: `smoller@umich.edu`